# Multiscale Mathematics for Materials

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Materials are enabling and limiting many of the technologies with high impact on our society (ranging from energy and environment to new nano- and bio-technologies).

Modeling and simulation are becoming increasingly important in materials science, as complement to experiment and as predictive tools for new systems with target properties. For example, in the last two decades, an increasing number of material properties have been simulated before any attempt was made to build specific devices (e.g. in the semiconductor industry).

The development of an interdisciplinary, multiscale math program to model and simulate materials is of paramount importance for progress in materials science. The great majority of materials science problems are inherently multiscale, encompassing length scales from the atomistic to the continuum and time scales from fs to sec. and to decades (e.g. in material aging and waste management problems). In addition a large body of work has been carried out in multiscale modeling of materials in the last decade, and new techniques have been developed (e.g. quasi-continuum models) showing the time is ripe for a sustained multi-math program for materials. This program will also bring key contributions to the tools needed to model matter at the nanoscale for emerging new nanotechnologies.

Investigation of specific materials (e.g. for fusion reactors) and high performance computing are among the major areas in the 20 year DOE roadmap. Therefore multiscale math for materials is not only greatly needed from a scientific standpoint, but it is a very timely initiative integrated within DOE long-range plan.

Science drivers for multiscale mathematics permeate all of materials science. We have identified some major scientific areas where the use of predictive multiscale capabilities can potentially lead to new discoveries by computer simulations. These areas are:

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- **Materials to go beyond CMOS technology,** including materials to realize molecular electronic devices and quantum computers.
- **Materials for fusion and fission reactors**, including materials resistant to radiation and other harsh environments.
- **Soft materials** for chemical and biosensors and for actuators, e.g. pi-conjugated polymers, and self-assembled structures.
- **Materials and processes for nuclear waste disposal,** including ion transport/exchange in cage materials and aqueous environments
- **Materials and chemical processes for clean energy sources,** e.g. materials for hydrogen storage and fuel cells.

Regarding material properties, we have identified the following challenging problems requiring multi-scale simulations: **fracture and failure**, **nucleation processes**,

**electronic and transport phenomena.** These are properties encompassing all of the materials categories identified above.

Some specific examples of materials science problems are given in the following, with a table illustrating the connection between the identified science drivers and the required developments in multiscale mathematics.

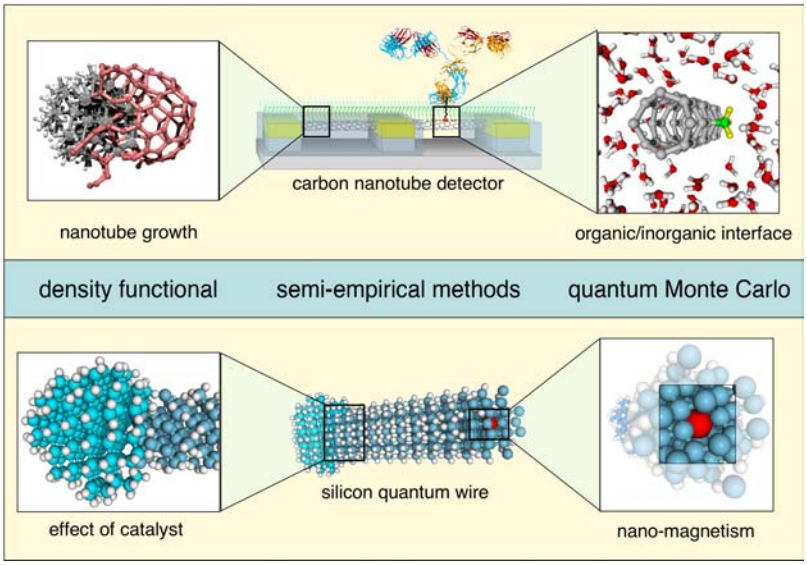
**--Nuclear waste migration** involves transport of a radioactive nuclide, e.g. Cs, out of the nuclear wasteform, e.g. a zeolite system, when the wasteform is in contact with ground water. The chemical process is believed to be cation exchange between the Cs and the Na in the ground water. Simulation of this rare event will involve reaction pathway sampling. Capturing the physics and chemistry which determine the ion exchange process will involve coupled quantum-classical-continuum simulations

**--Nucleation and self-assembly of quantum dot arrays** produces nanoscale systems, but their use in microelectronics and other applications is critically dependent on achievement of uniformity in their size, shape and spacing. Simulation of the initial wetting layer, nucleation and self-assembly will require simulation at the atomistic, single dot and multiple dot length scales.

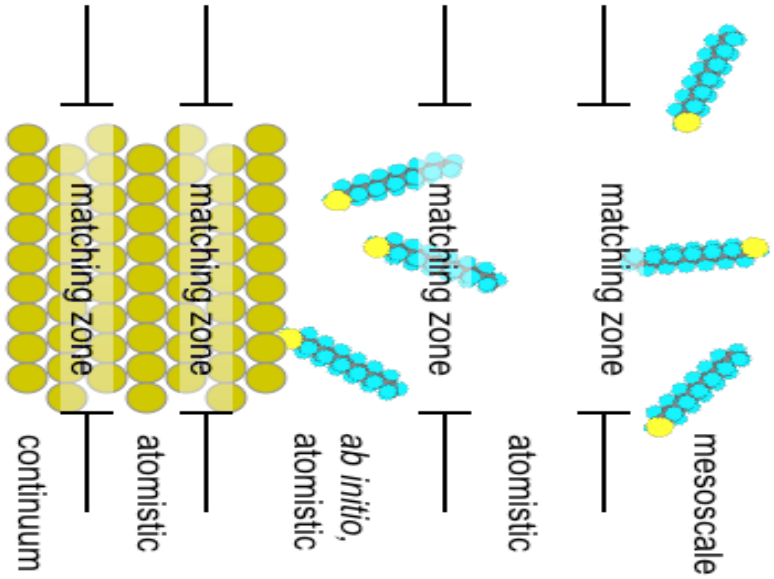
**--Design of novel materials with specific sensing and labeling properties** requires the simulation of interfaces between inorganic surfaces and organic matter in the presence of a wet environment and the study of reaction paths between organic molecules and inorganic probes (see Fig.1). This involves atomistic simulations both at the quantum and effective potential level, coupled with continuum description of, e.g. a solvent, and the simulations of both rare events and equilibrium phenomena over time scales from ps to ns.

| | Coupling of length scales | Coupling of time scales | Major Challenging properties |
|---|---|---|---|
| **Beyond CMOS** | Quantum-Quantum (e.g. DFT/QMC) Quantum-Classsical (QM/MM) | Accelerated dynamics for both classical and quantum molecular dynamics (MD) | Nucleation, electronic and transport |
| **Materials for Fusion** | Quasi-continuum models for MD | Beyond ns time scales in MD | Fracture and failure, resistance to radiation |
| **Soft Materials** | Quantum-Classical-Continuum | Accelerated dynamics for quantum methods | Electronic and transport |
| **Nuclear Waste** | Quasi-continuum coupled to quantum-classical models | Rare events and beyond ns time scales in MD | Electronic and transport; fracture and failure |
| **Clean Energy** | Quantum-Quantum Quantum-Classsical (QM/MM) | Accelerated dynamics for both quantum and classical methods | Electronic and transport |

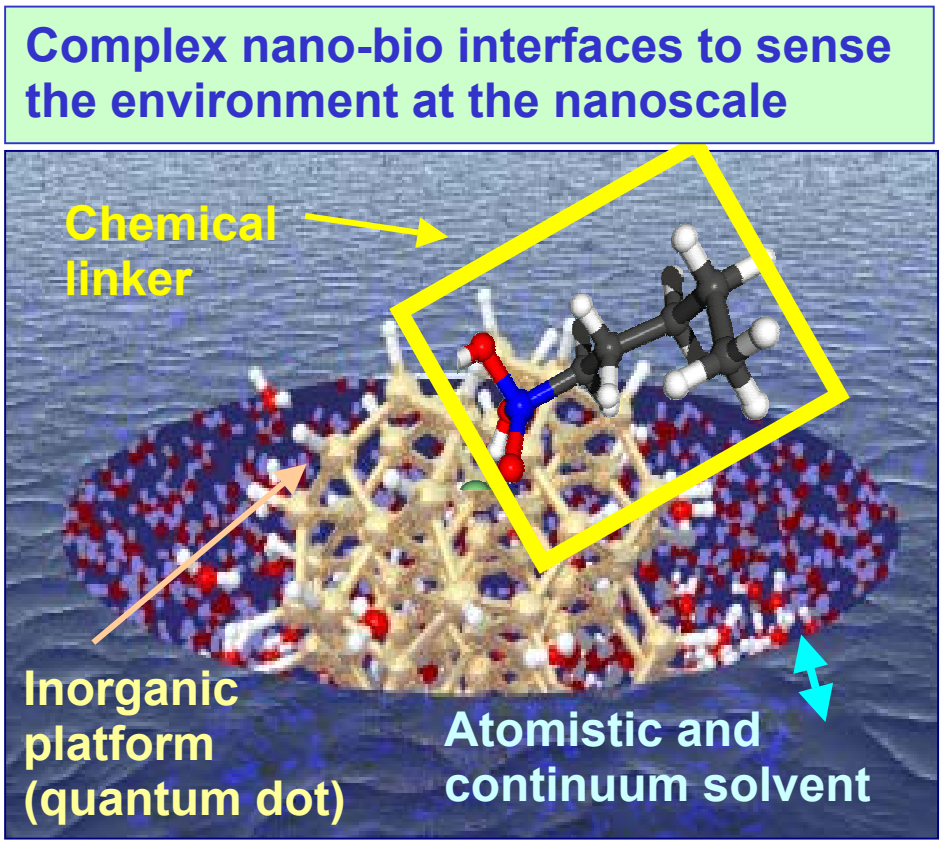
Examples of pictures related to the problems outlined above are given below.



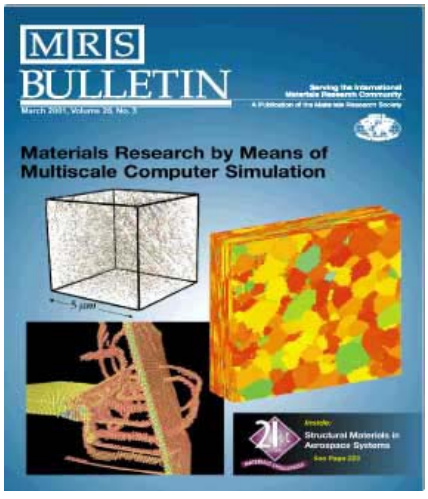

This figures illustrates how nano-materials for sensing (upper panel) or electronic (lower panel) applications (see areas "Beyond CMOS" and "Soft Matter") can be described with different quantum mechanical and semi-classical models which provide different levels of accuracy and whose coupling bridge length scales from A to tens of nm.




*A muliscale approach to the simulation of molecular devices (Cummings, Harrison et al.)*




This figure illustrates how an inorganic platform to sense the environment is linked to a chemical agent in an aqueous solution. Coupling of different quantum mechanical methods, of quantum to classical and finally to continuum models are required to study the sensing properties of this system in the appropriate wet ambient.




A recent cover of the MRS bulletin, focused on Materials Research by means of multi-scale computer simulations, illustrating some dislocation dynamic simulations and mesoscopic modeling of materials